

Large Language Models to Enhance Bayesian Optimization

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Abstract

Bayesian optimization (BO) is a powerful approach for optimizing complex and expensive-to-evaluate black-box functions. Its importance is underscored in many applications, notably including hyperparameter tuning, but its efficacy depends on efficiently balancing exploration and exploitation. While there has been substantial progress in BO methods, striking this balance remains a delicate process. In this light, we present LLAMBO, a novel approach that integrates the capabilities of Large Language Models (LLM) within BO. At a high level, we frame the BO problem in natural language, enabling LLMs to iteratively propose and evaluate promising solutions conditioned on historical evaluations. More specifically, we explore how combining contextual understanding, few-shot learning proficiency, and domain knowledge of LLMs can improve model-based BO. Our findings illustrate that LLAMBO is effective at zero-shot warmstarting, and enhances surrogate modeling and candidate sampling, especially in the early stages of search when observations are sparse. Our approach is performed in context and does not require LLM finetuning. Additionally, it is modular by design, allowing individual components to be integrated into existing BO frameworks, or function cohesively as an end-to-end method. We empirically validate LLAMBO's efficacy on the problem of hyperparameter tuning, highlighting strong empirical performance across a range of diverse benchmarks, proprietary, and synthetic tasks.